Corner transfer matrix renormalisation group method for two-dimensional self-avoiding walks and other $O(n)$ models

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We present an extension of the corner transfer matrix renormalisation group (CTMRG) method to $O(n)$ invariant models, with particular interest in the self-avoiding walk class of models ($O(n=0)$). The method is illustrated using an interacting self-avoiding walk model. Based on the efficiency and versatility when compared to other available numerical methods, we present CTMRG as the method of choice for two-dimensional self-avoiding walk problems.

The self-avoiding walk class of models on the two-dimensional square lattice, with a variety of possible interactions, has mobilised the scientific community for about half a century[1, 2]. The number of exact results for such models is limited, and numerical studies are hard. A clear illustration of the numerical difficulty is the disagreement which existed over the numerical determination of critical temperature and exponents for the standard θ-point model, see for example references[3].

To date the numerical methods available for the study of interacting self-avoiding walks in two dimensions are series expansions of walks of lengths of a few tens of steps[4], transfer matrices for lattice widths up to about 12[5] and increasingly complicated Monte-Carlo simulation methods[6], limited in practice to only a portion of the phase diagram.

Motivated by these numerical difficulties, we decided to extend the Corner Transfer Matrix Renormalisation Group (CTMRG) method[7]. The CTMRG method is based on White's Density Matrix Renormalisation Group method (DMRG)[8] and Baxter's corner matrix formalism[9]. To date the CTMRG method has only been applied to discrete spin models, where it is shown to be computationally efficient[7].

Our extension to interacting self-avoiding walk models exploits the connection betweeen these models and the $O(n)$ invariant spin models[10], which contains as special cases the Ising model ($n=1$), the XY model ($n=2$) and the Heisenberg model ($n=3$). The method therefore has applications well beyond the self-avoiding walk type models ($n=0$).

The $O(n)$ spin model is defined through the partition function[11]

$$\mathcal{Z}_{O(n)} = \sum_{\{\vec{s}_i\}} \exp\left(\frac{1}{2}\beta J \sum_{\langle i,j\rangle} \vec{s}_i \cdot \vec{s}_j\right), \qquad (1)$$

where $\langle i,j\rangle$ refers to a sum over nearest neighbour spins. The spin $\vec{s}_i$ has n components, and is normed such that $s_i^2 = 1$. Another formulation of $O(n)$ invariant models, with the same critical behaviour, is:

$$\mathcal{Z}_{O(n)} = \sum_{\{\vec{s}_i\}} \prod_{\langle i,j\rangle} (1 + K\vec{s}_i \cdot \vec{s}_j). \qquad (2)$$

where the spins are now placed on the lattice bonds[10]. A diagrammatic expansion of Equation 2 follows if we identify the 1 as the weight of an empty bond between the sites i and j and the K as the weight of an occupied bond. This expansion may be expressed in terms of graphs $\mathcal{G}$ of non-intersecting loops (collisions at sites are however allowed)[10]. The partition function may then be written:

$$\mathcal{Z}_{O(n)} = \sum_{\mathcal{G}} n^{l(\mathcal{G})} K^{b(\mathcal{G})}, \qquad (3)$$

where l is the number of loops and b is the number of occupied bonds.

The parameter n is now a fugacity controlling the number of loops, and need no longer be taken as an integer. This fugacity corresponds to a long ranged interaction, since the loops may be of any size. This non-locality is undesirable for our purposes. We would like to express n as a product over local weights. This may be achieved as follows. Each loop may be followed clockwise or anticlockwise. The loops in Equation 3 are not oriented, but may be oriented by associating $2^{l(\mathcal{G})}$ oriented graphs with each non-oriented graph. By associating a loop fugacity n_+ (n_-) with the clockwise (anticlockwise) oriented loops, the partition function may be rewritten[12]:

$$\mathcal{Z}_{O(n)} = \sum_{\mathcal{G}} (n_+ + n_-)^l K^b = \sum_{\mathcal{G}'} n_+^{l_+} n_-^{l_-} K^b \qquad (4)$$

where $\mathcal{G}'$ is the set of oriented loop graphs, and l_+ (l_-) is the number of clockwise (anticlockwise) oriented loops. Setting $n_+ = \exp(i\theta)$ and $n_- = \exp(-i\theta)$ gives $n = 2\cos(\theta)$. The oriented loop factor is now broken up into local weights by associating a corner weight $w_i = \exp(i\theta/4)$ with every clockwise corner and $w_i = \exp(-i\theta/4)$ with every anticlockwise corner. On the square lattice, there must be four more corners with one orientation, compared with the other orientation, in order to close a loop. The product of the local weights will then give the correct weight for the oriented loops.

The partition function may now be rewritten in terms of a vertex model[10]:

$$\mathcal{Z}_{O(n)} = \sum_{\mathcal{G}'} \prod_i v_i \qquad (5)$$

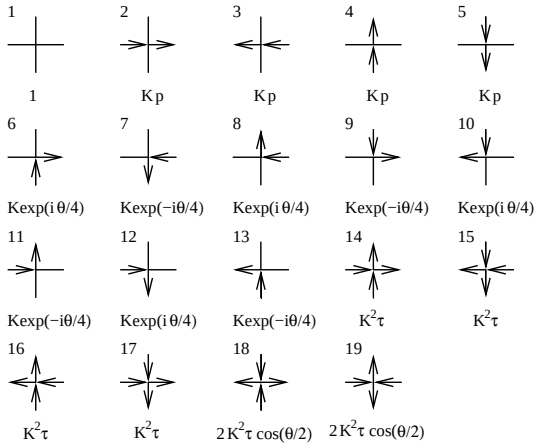

FIG. 1: The 19 allowed vertices in the most general $O(n)$ model. K is the step fugacity and $\tau = \exp(-\beta\epsilon)$, where ϵ is the attractive monomer-monomer interaction energy.

where v_i is the weight of the vertex at site i. The derivation given here is only for the simplest case, but we may freely change the weights of the vertex configurations in order to generate different interactions in the original model (see figure 1).

The limit $n \to 0$ corresponds to the self-avoiding walk model[13]. In the generalised form presented here this corresponds to an interacting self-avoiding walk model due to Blöte and Nienhuis[10, 14]. A step fugacity K and an attractive short ranged interaction $\varepsilon < 0$ are introduced. In the standard θ point model the interactions are between non-consecutively visited nearest-neighbour sites and a given site may only be visited once[1, 2]. In our current models, this last constraint is relaxed; the walk may collide at a site, but not cross, and remains self-avoiding for the bonds. The interaction is now assigned to doubly visited sites. An additional weight p is added for sites which are visited by a straight section of walk (i.e. do not sit on a corner). The partition function may then be written:

$$Z = \sum_{\text{walks}} (Kp)^L \tau^{N_I} p^{-N_c}, \tag{6}$$

where $\tau = \exp(-\beta\varepsilon)$, N_I is the number of site collisions and N_c are the number of corners in the walk. This model gives rise to the vertex weights shown in figure 1. The standard self-avoiding walk model is found setting $\tau = 0$ and $p = 1$ and when $p = 0$ the model has the same critical behaviour as the standard θ point model[14]. During the remainder of this letter we shall illustrate the CTMRG method for $O(n)$ models using this Blöte-Nienhuis walk model.

Following Baxter[9], the partition function of a two dimensional lattice model may be written in terms of the product of four matrices representing the four quarters of the lattice. The inputs and outputs of the matrices are the configurations at the seams of the four quarters. These matrices are known as corner transfer matrices. In general the four matrices are different, but may often be related by lattice symmetries. For our model the four matrices are the same up to a complex conjugation operation[16].

It is usually not possible to calculate explicitly these matrices for systems with a large number of sites. This is where the CTMRG method comes in; the matrices for larger lattices are calculated from smaller lattices iteratively[7]. This is done as follows. An initial system, consisting of a small number of sites, is mapped exactly onto a prototype system made up of four m-state spins. At each iteration the system is enlarged by adding sites, this enlarged system is then projected back onto the prototype system in some optimal way, so as to minimise the loss of information. The value of m determines the amount of information which may be carried forward at each iteration, the larger the value of m the better the approximation. For details see [7, 16].

As with the DMRG method, the innermost sites of the lattice are treated exactly. This means that the CTMRG method is most appropriate for the calculations of one-point functions such as the site free energy, the site density of monomers, specific heats etc. In figure 2 we show the density, ρ, as a function of the step-fugacity K for fixed values of τ. We chose to fix $p = 0$ since for this value the Nienhuis-Blöte model has the same critical behaviour as the standard θ point model[14]. When $\tau < 2$ the model is expected to be in the self-avoiding walk universality class and present a critical transition where the density changes continuously from $\rho = 0$ for $K < K_c$ to $\rho > 0$ for $K > K_c$. When $\tau = 2$ the transition is expected to be tricritical, in the same universality class as the θ point, with $K_c = 1/2$ exactly. For $\tau > 2$ the transition is expected to be first order. These three types of behaviour may be clearly seen in figure 2.

Whilst the raw finite-size data presented in figure 2 already gives a fairly precise idea of the behaviour of the system (order of the transition and first estimate of K_c), practical calculations of critical temperature and critical exponent estimates rely on finite-size analysis. In transfer matrix calculations one usually uses a phenomenological renormalisation group based on the correlation lengths due to Nightingale[15]. In the CTMRG method an effective transfer matrix may be determined directly. However, as already mentioned, the highest precision is obtained for the one point correlation functions. Since the number of sizes available is an order of magnitude larger than that available for transfer matricies it is advantageous to exploit the finite size scaling laws for the one point functions. In particular it is expected that the singular part of the density scales as

$$\rho_s(K, L) = L^{1/\nu - 2} \tilde{\rho}(|K - K_c| L^{1/\nu}). \tag{7}$$

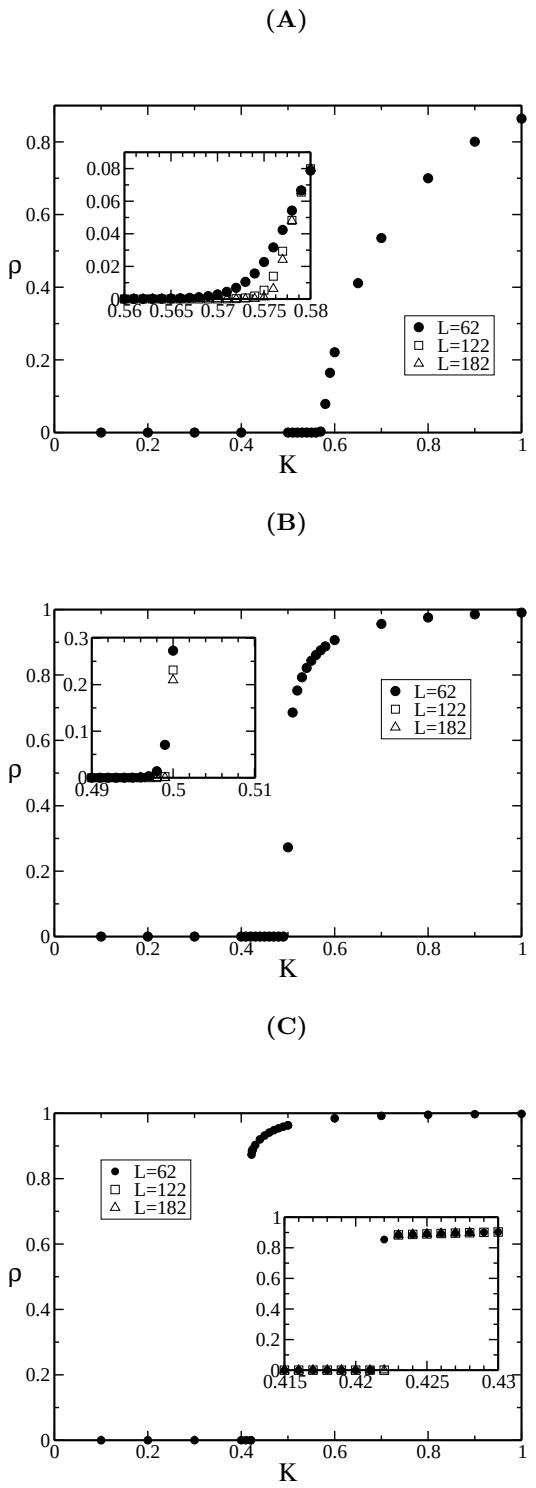

FIG. 2: The density, ρ, as a function of K with $p = 0$ and (A) $\tau = 1$, (B) $\tau = 2$ and (C) $\tau = 3$ for $L = 62, 122$ and 182. Estimates of K_c from finite size scaling are given in table I. The value of K for the first order transition when $\tau = 3$ estimated directly from the jump in the density was found to be $K^* = 0.422 \pm 0.001$ (compared to 0.421 ± 0.001 found previously[14]).

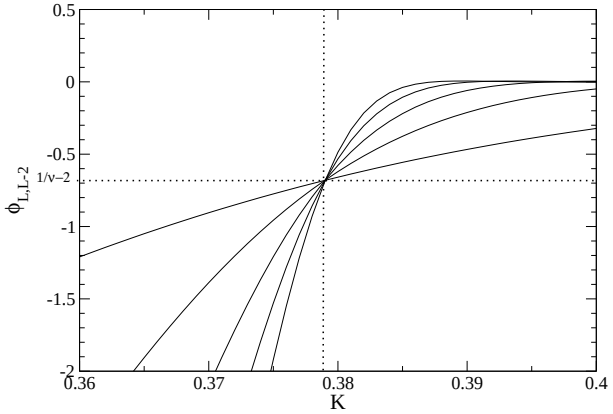

FIG. 3: $\varphi_{L,L-2}$ as a function of K for the self-avoiding walk model ($p = 1$, $\tau = 0$) for $L = 10, 20, 30, 40$ and 50. The horizontal and vertical lines give the corresponding finite size estimates of K_c and ν.

This scaling behaviour implies that the function

$$\varphi_{L,L'}(K) = \frac{\log\left(\rho_s(K,L)/\rho_s(K,L')\right)}{\log\left(L/L'\right)} \tag{8}$$

takes the value $\varphi_{L,L'} = 1/\nu - 2$ when $K = K_c$, independantly of L and L'. Naturally there are additional finite size corrections which should be taken into account, but the conclusion is that if the function $\varphi_{L,L'}(K)$ is plotted for various values of L and L' then it will converge to a fixed point given by $\varphi(K_c) = 1/\nu - 2$. In what follows we have set $L' = L - 2$ and looked for solutions of the equation

$$\varphi_{L,L-2}(K_c^L) = \varphi_{L-2,L-4}(K_c^L), \tag{9}$$

where K_C^L is the estimated critical temperature from sizes L, $L-2$ and $L-4$. If such a solution does exist then $K_c = \lim_{L\to\infty} K_c^L$ and $\nu = \lim_{L\to\infty} 1/(\varphi_{L,L-2}(K_c^L) - 2)$.

Figure 3 shows φ plotted for several values of L for the pure self-avoiding walk model ($p = 1$, $\tau = 0$). The different curves cross at a point defining K_c and ν. The corresponding estimates of K_c and ν are shown in Figure 4 plotted as a function of $1/L$. The extrapolations of K_c^L and ν^L to $L \to \infty$ are given in Table I along with prelimenary estimates for $p = 0$ and different values of τ. The accuracy with which the critical points are determined is in general an order of magnitude better than found with transfer matricies. Full details and definitive estimates will be given elsewhere [16].

In (numerically) exact methods, such as the transfer matrix method or the exact enumeration method, the main source of uncertainty in the results is due to the extrapolation of a small number of points. In the CTMRG method the extrapolation problems are largely removed since lattice sizes an order of magnitude larger have been reached. The uncertainty now lies in the precision related to the calculation of each density point.

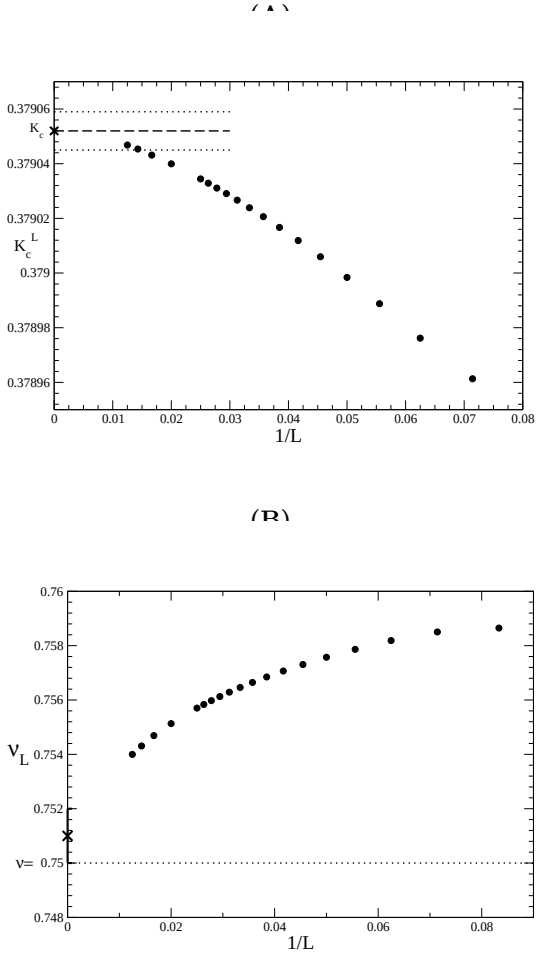

FIG. 4: (A) Critical point and (B) critical exponent estimates for the self-avoiding walk ($p = 1$, $\tau = 0$) as a function of $1/L$. The extrapolated values of K_c and ν are shown. In (A) the three horizontal lines show the previous transfer matrix estimate for K_c along with the corresponding error bars[2]. In (B) the horizontal dotted line indicates the exact value of $\nu = 3/4$.

In this article results for the Blöte-Nienhuis interacting self-avoiding walk are presented since good quality results already exist, providing a good test of the efficiency of the CTMRG method. In particular we have focused on the self-avoiding walk model ($p = 1$, $\tau = 0$) for which the asymptotic limit is well described by transfer matrix calculations and yet we still find a substantial increase in precision (see Table I). It is clear that in circumstances where larger system sizes are required to extract the scaling behaviour, CTMRG should far exceed the numerically exact methods in performance.

The quality of results presented in this article is virtually unattainable with such ease by any other numerical method we know of (there is a very small number of exceptional cases where better accuracy was obtained[17]) and so we present CTMRG as the method of choice for two-dimensional self-avoiding walk models. CTMRG may easily be extended to more complicated interacting self-avoiding walk models, such as the hydrogen-bonding self-avoiding walk[18].

p	τ	TM K_c	CTMRG K_c	ν
0	0	0.63860 ± 0.00005	0.63865 ± 0.00005	0.755 ± 0.007
0	1	0.5769 ± 0.0001	0.57686 ± 0.00002	0.74 ± 0.02
0	2	0.5001 ± 0.0001	0.500000 ± 0.000001	0.571 ± 0.001
1	0	0.379052 ± 0.000007	0.379052 ± 0.000001	0.751 ± 0.001

TABLE I: Estimates of K_c from transfer matrix (TM) calculations taken from reference [14] for $p = 0$ and from reference[2] for the self-avoiding walk ($p = 1$ and $\tau = 0$) are compared to our (previsional) estimates using the CTMRG. First estimates of ν using CTMRG are also given.

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